



Recent progress on Labfit: a robust multispectrum analysis program for fitting lineshapes including the HTP model and temperature dependence

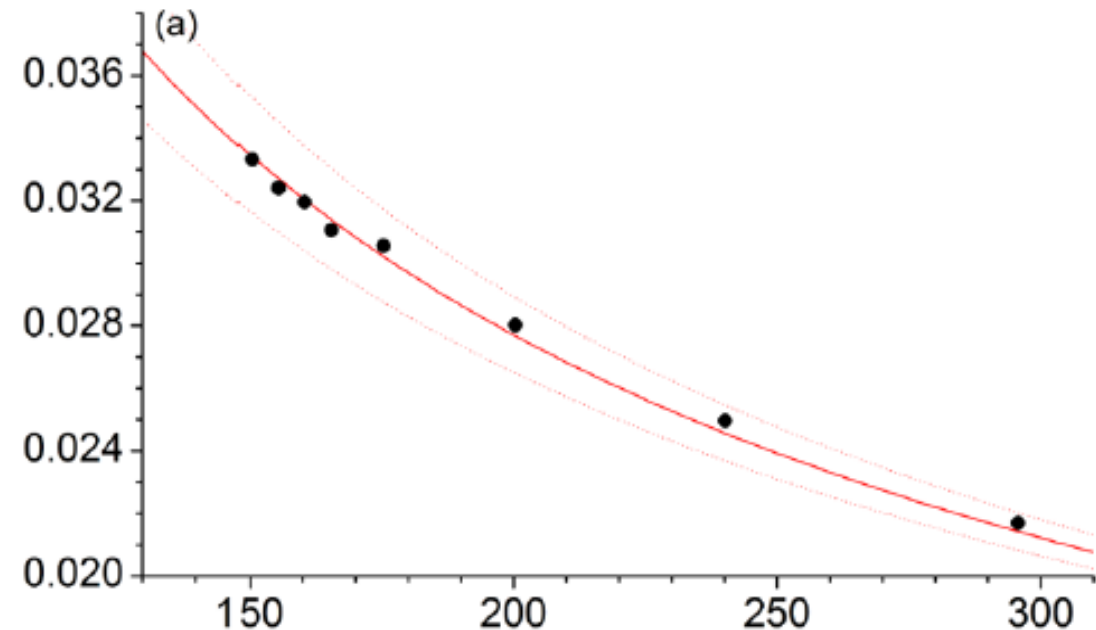
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Why is Multispectrum Fitting Important?

- Reducing Correlations between parameters and finding true physical values rather than just getting a good fit.
- Ideally, the fit receives information from a variety of temperatures and pressures to contribute to parameter values
- With high signal-to-noise data, accurate fitting of higher order parameters is very difficult or impossible without a multispectrum approach.



What is Labfit?

A highly versatile multispectrum fitting tool

- Originally developed in Fortran as a text-based tool by Chris Benner for Kit Peak FTS spectra. It has been used in numerous publications starting in ~1995
- ~2013 the code was modernized, and an external Python GUI was added
 - Alexandre Guillaume, Brian Drouin, Kyle Dodge, Caitlin Bray, etc...
 - Binary spectrum support remains but ascii-formatted support was added

```
Ch=|Eh=|:h=äyg=:çg=™Ch=X-  
h=◊h=ö/h=YËh=çžh=E7h=±  
%h=ŽRh=↑yh=|Rh=ü[h=|h=òh=õ~g=Æ)  
h=}uh=óh=ê•h=çMh=%vh=M\h=|f  
h=S'h=İeh=Z$h=®*h=0eh=7
```

or

```
***** AIR CRDS 1000 Torr  
3905 13023.1518850000 13031.264414000 0.0067379808  
100000.00 0.00000 6.00e-8 7 22 41  
10000.0000000 21.3838 985.4548 0.207200  
0.0000000 23.1587 0.00000 0.000000  
0.0000000 23.1587 .000000 .000000  
1. 1. 1. 1. 1. 1. 1. 1. 1. 1.  
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```

- The GUI-Based Labfit is now available for use and almost user-friendly
- What features does Labfit have?

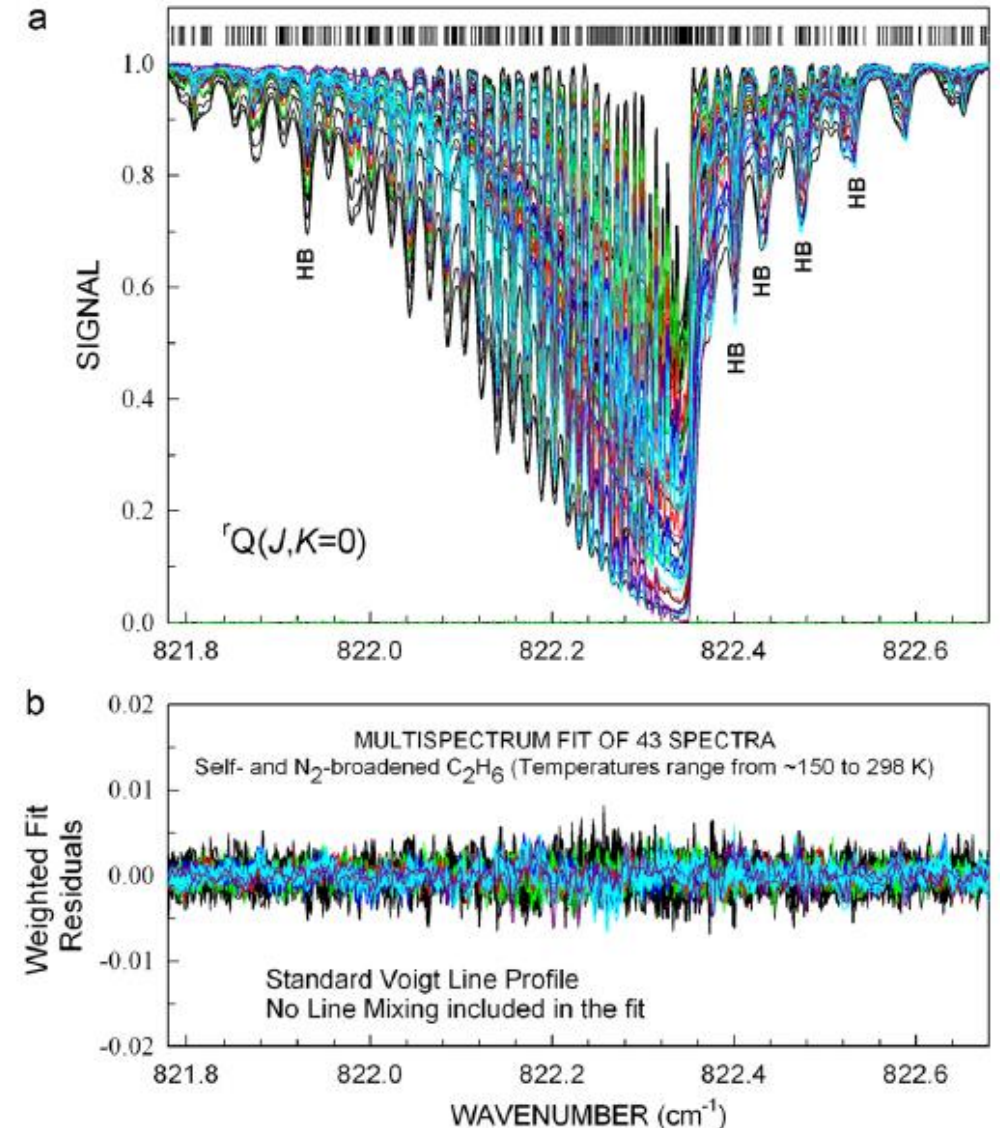
Labfit Features: Text-based Labfit

Ethane Q Branch at 822 cm^{-1}

Major Highlights:

- 43 FTIR spectra
- Voigt line shapes

Devi et al.: doi:10.1016/j.jqsrt.2010.07.010

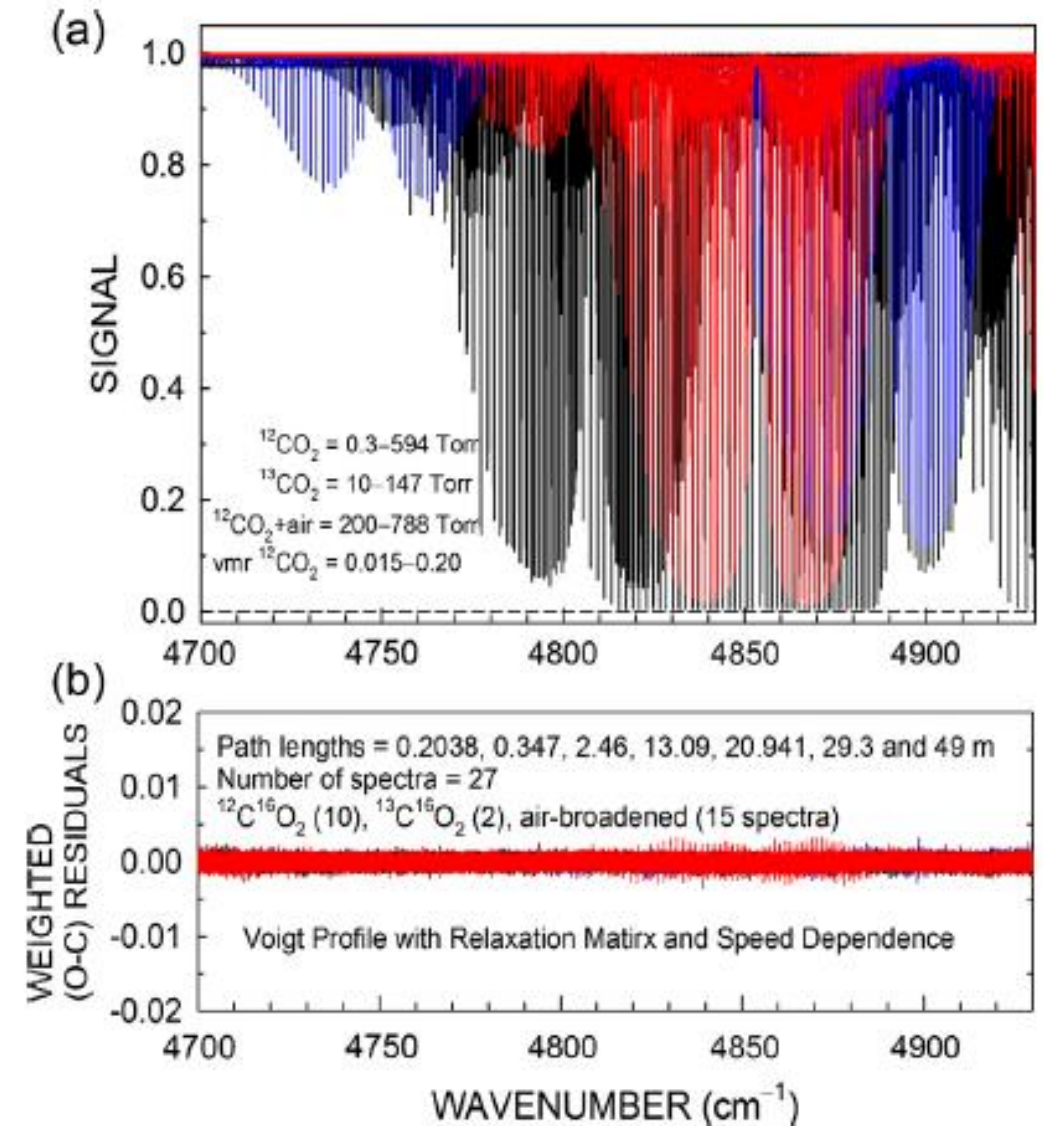


Labfit Features: Text-based Labfit

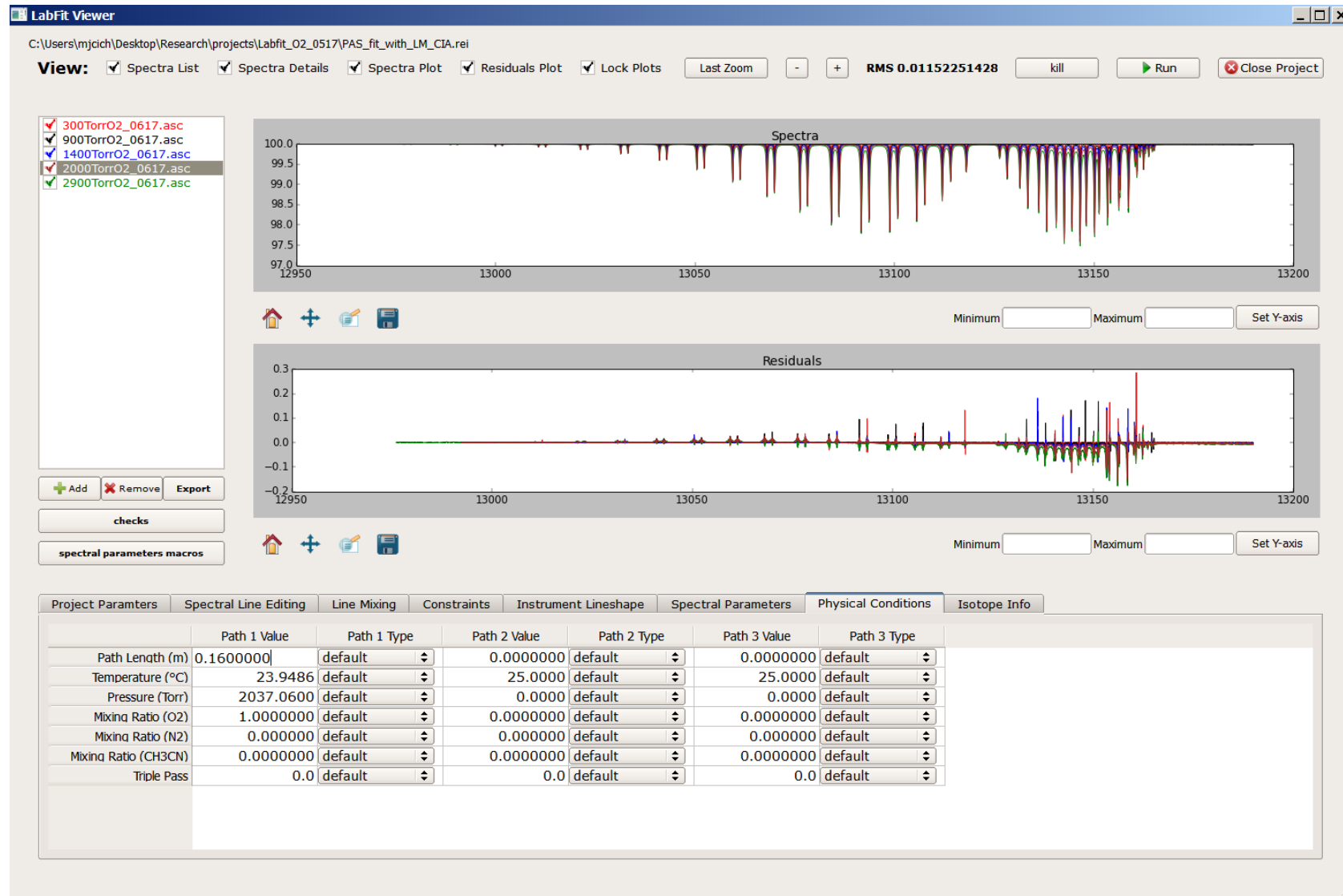
CO₂ fit for OCO-2 at 4700-4930 cm⁻¹

Major Highlights:

- Speed-Dependent Voigt (SDV)
- ~600 lines fit (112 SDV)
- 170K-296K temperatures
- Matrix-formalism line mixing
 - (Rozenkranz parameters are available)
- 4 isotopes observed



Labfit Features: GUI



Labfit Features: Handling a Variety of Spectra

- Many instrument lineshape features for FTIR
- Baseline: multi-termed polynomial useful for a variety of instruments

Spectral Line Editing Line Mixing Constraints **Instrument Lineshape** Spectral Parameters Physical Conditions

Maximum Optical Path Difference (FTS 0.9/Bruker Resolution) Fixed

Omega (FTS Field of View $\pi \cdot r^2 / f^2$, $\pi \cdot r(\text{mm})^2 / 418^2$) Fixed

Effective Apodization Fixed

Phase (degrees) Fixed

Background Parameters

☐ show background

Edit Background Parameters

Background Parameters

	Value	Type
1	0.907014000...	float
2	-0.063306200...	float
3	0.011064500...	float
4	-0.001322310...	float
5	-0.000716045...	float
6	-0.001126450...	float
7	-0.000287693...	float
8	0.000280669...	float
9	0.000143886...	float

Labfit Features: Handling a Variety of Spectra

- Additional options such as wing cutoff, etalons, and frequency calibration factors
- Also has mixing ratios for 3 gasses in up to 3 paths and isotope enhancements for up to 18 isotopes (thanks to CO₂).

Parameters	Spectral Line Editing	Line Mixing	Constraints	Instrument Lineshape	Spectral Parameters	Physical Conditions	Isotope Info
Run #:		4658		Unknown Fixed 9.99999			
Initial Freq. (cm⁻¹):		12950.0		Zero Fixed 0.0			
Final Freq. (cm⁻¹):		13190.0		Wing Cut Off 0.0001			
Freq. Spacing (cm⁻¹):		0.005		Weight 1.0			
Spectrum Type:				Channel <input type="text"/> <input type="button" value="Add Channel"/>			
CRDS:				<input type="text"/> <input type="text"/> <input type="text"/>			
Cal Factor x		<input type="text" value="-3000.0"/>	Fixed	<input type="text" value="Float"/> <input type="text" value="Float"/> <input type="text" value="Float"/>			
Cal Factor +		<input type="text" value="0.0"/>	Fixed				
				RMS 0.191281083453			
				Amplitude Period Phase			

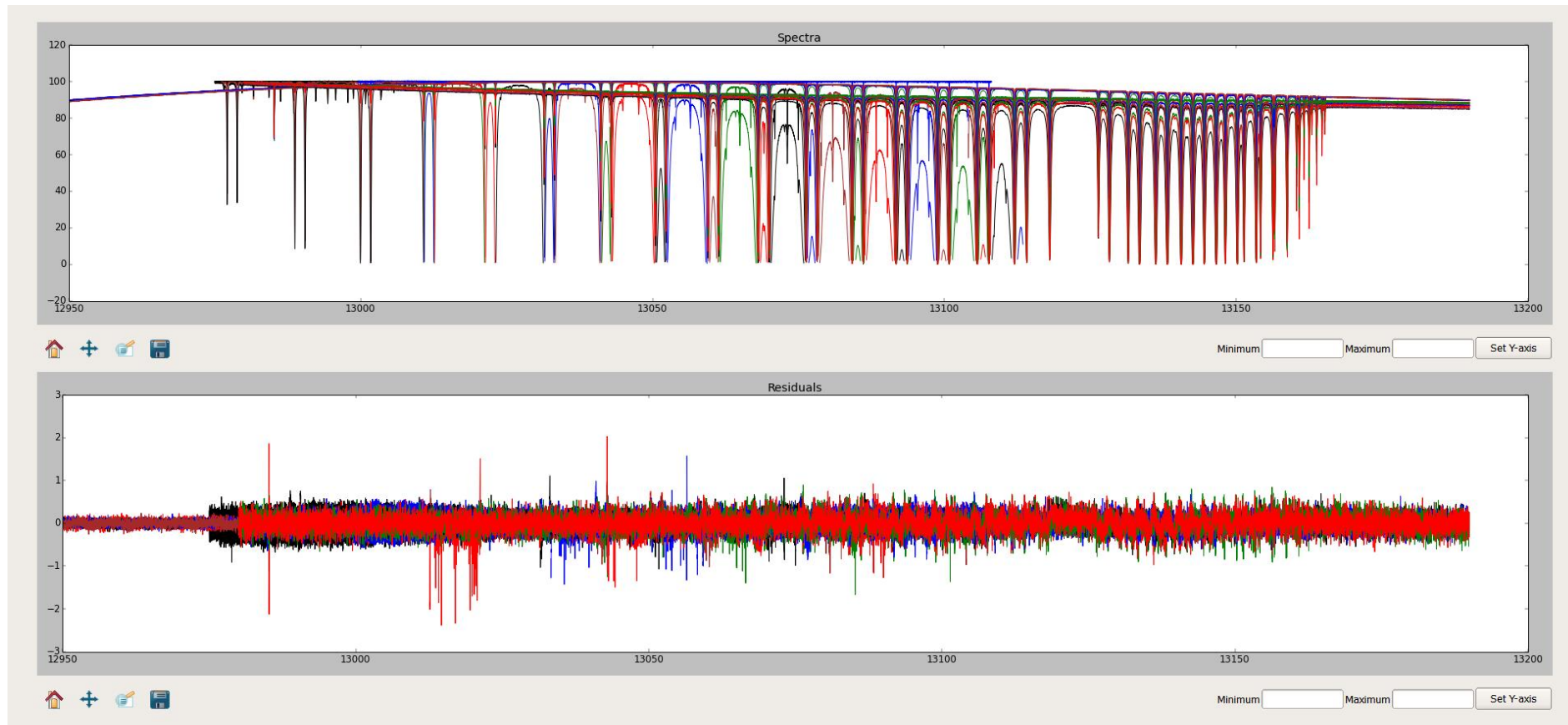
Labfit Features: Line List

- Ability to fix or float lineshape parameters in a sortable line-by-line list
- Can block select, add and delete lines
- Accepts HITRAN formatted line lists as an input option

[illegible]

Labfit Features: OCO-2 O₂ A-band Fit

- Takes data from FTIR (binary) and cavity ring-down (ascii) simultaneously
- Collision-induced absorption and line mixing (matrix)



Labfit Features: A-band fit (2)

Project Parameters Spectral Line Editing Line Mixing Constraints Instrument Linesh...

Auxiliary Parameters ☒ show auxilliary parameters 500 limit Add Auxiliary Parameter

40	G'-E0-?	0.1312200603D+05	float	▴ ▾
41	B'	0.1391247654D+01	float	▴ ▾
42	D'	0.5363091927D-05	float	▴ ▾
43	H'	-0.8709244657D-11	float	▴ ▾
44	LM RQ foreign ...	-0.5000000000D+00	fixed	▴ ▾
45	LM RQ self scale	-0.5000000000D+00	fixed	▴ ▾

- Constraints and auxiliary parameters allow for broad fitting options
- Math operations $+$, $-$, \times , \div , $^$, etc. have derivatives coded in for general cases to allow for user-defined fitting rules.
- Line positions, intensities, or other known relations between lines

Initial Parameters Physical Conditions Isotope Info

operation ▴ ▾ case b ▴ ▾ Add Constraints O2 ▴ ▾ 1 ▴ ▾

Initial Auxiliary Parameter 10 P ▴ ▾ Auxiliary Parameter 1 ▴ ▾

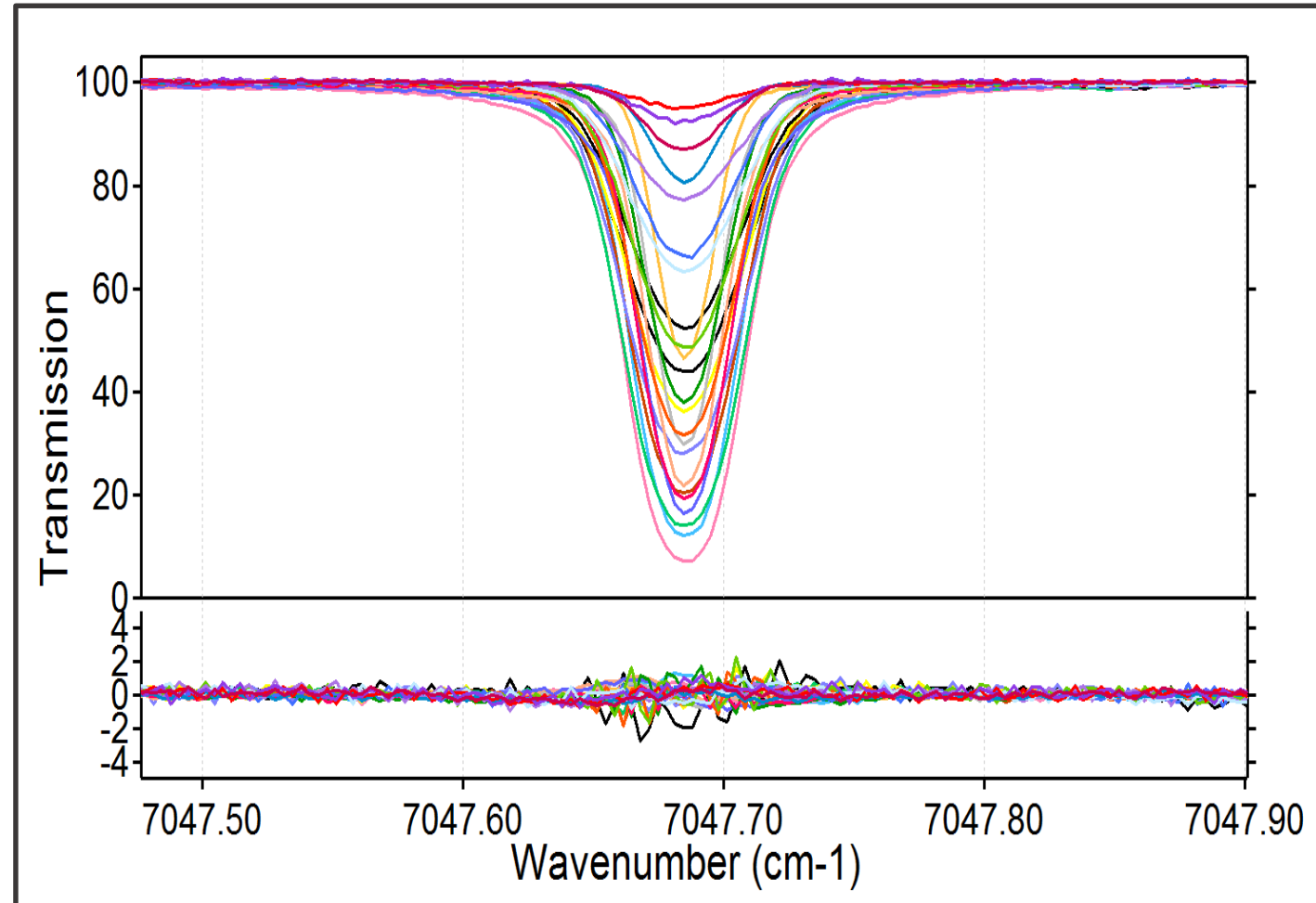
Quantum character location 18 vibronic string + ▴ ▾ Auxiliary Parameter 1 ▴ ▾

Minimum line # 0 Minimum wavenumber 0 Auxiliary Parameter 1 ▴ ▾

Maximum line # 50000 Maximum wavenumber 20000 Increment all 0 ▴ ▾

Labfit Features: Hot Water

- See next talk! ([WJ09](#))
- 25 spectra over a large temperature range
- Proof that it is “user friendly”
- Constraints and auxiliary parameters used to resolve complicated overlapping lines



Schroeder PJ, Pfortenhauer DJ, Yang J, Giorgetta FR, Swann WC, Coddington I, et al. High temperature comparison of the HITRAN2012 and HITEMP2010 water vapor absorption databases to frequency comb measurements. JQSRT 2017.

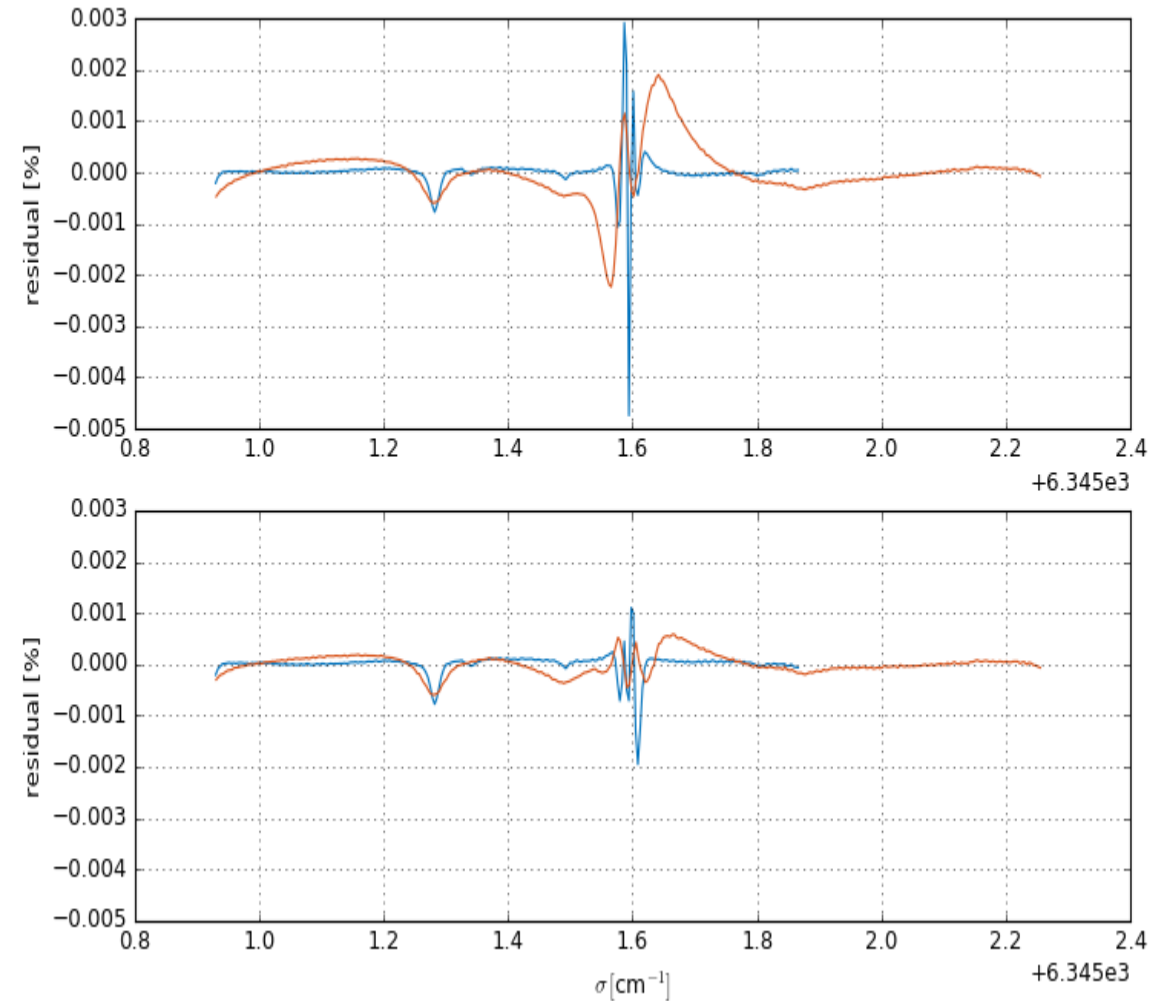
Labfit Features: Coming Soon

Hartmann-Tran Profile (HTP) has been added (Alexandre Guillaume)

- Provides updates to Labfit's parameters to make them more compatible with gas mixtures and temperature dependence

Analytical derivatives still being added

Test fit of 2 spectra of CO data* shows that the coded HTP results in an improvement over the previous model.



*JT Hodges, ZD Reed, NIST Gaithersburg, MD. private communication 3/2017

Summary

- Can fit a wide variety of experimental spectra, with many lines, temperatures and pressures with a large number of baseline options
- Useful for fitting high order line shapes, with CIA, LM and soon HTP.
- Versatility with many baseline options and user-defined constraints
- Available for PC, Mac, and Linux!
- **How to obtain: contact Brian Drouin or go to download.jpl.nasa.gov**
- The End

- **Thank you to the many authors of the studies shown for your figures and support!**
- This work was supported by the National Aeronautics and Space Administration (NASA). Part of the research was performed at Jet Propulsion Laboratory (JPL) under contract with NASA.

